

Phonon Tunneling Loss Solver for Micro- and Nanomechanical Resonators

Garrett D. Cole^{*†,1}, Ignacio Wilson-Rae², and Markus Aspelmeyer¹

¹ Universität Wien, ²Technische Universität München

*Corresponding author: Boltzmanngasse 5, Vienna, A-1090, Austria, garrett.cole@univie.ac.at

Abstract: Micro- and nanoscale mechanical resonators have emerged as ubiquitous devices for application in a wide range of technical disciplines including communications, sensing, metrology, and fundamental scientific endeavors. In many instances the performance of these devices is limited by the deleterious effects of mechanical damping. To further compound this limitation, the quantitative understanding of these damping mechanisms remains elusive in many cases. Here, we report a significant advancement towards predicting and controlling support-induced losses, a key dissipation mechanism in high-quality-factor mechanical resonators. Utilizing COMSOL multiphysics, we have developed an efficient FEM-enabled solver, employing the recently introduced “phonon-tunneling” approach. With this solver we demonstrate the ability to predict the design-limited damping of generic mechanical resonators, yielding excellent agreement with experimental measurements. Thus, our phonon-tunneling solver represents a major step towards accurate prediction of the mechanical quality factor in micro- and nanomechanical resonators.

Keywords: damping, mechanical resonators, MEMS/NEMS, quality factor.

1. Introduction

Although much progress has been made towards the understanding of mechanical dissipation at the micro- and nanoscale [1,2], obtaining reliable predictions of the fundamental design-limited quality factor, Q , remains a major challenge. The origins of mechanical damping in micro- and nanoscale systems have been the subject of numerous studies, with several relevant loss mechanisms having been investigated [1,2]. These include: (i) fundamental anharmonic effects such as phonon-phonon interactions [1,3], thermoelastic damping (TED) [1,3-6], and the Akhiezer effect [1,3]; (ii) viscous damping, involving interactions with the surrounding atmosphere or the compression of

thin fluidic layers [7-9]; (iii) materials losses driven by the relaxation of intrinsic or extrinsic defects in either the bulk or surface of the resonator [10-14] for which the most commonly studied model is an environment of two-level fluctuators [15,16] and (iv) support-induced damping, i.e. the dissipation induced by the unavoidable coupling of the resonator to the substrate [17-21], which is typically referred to as anchor [17] or clamping [2] loss in the literature and corresponds to the radiation of elastic waves into the supports [22-27].

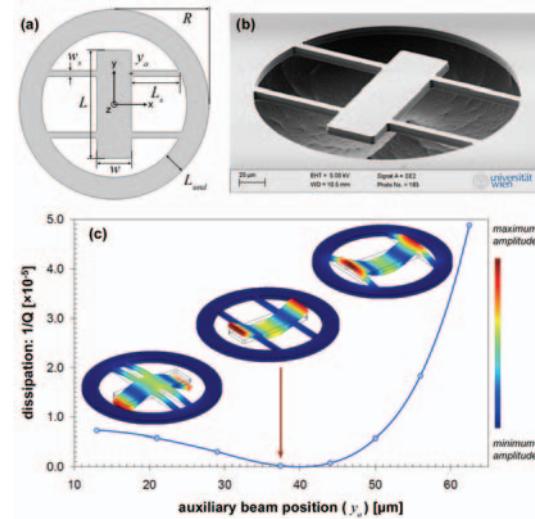


Figure 1. Mapping out phonon-tunneling dissipation in a free-free resonator. (a) Schematic diagram of the resonator geometry. (b) Scanning electron micrograph highlighting a single suspended structure. (c) Simulated dissipation [cf. Eq. 1] as a function of the y -coordinate (y_a) of the auxiliary beam. Values corresponding to 8 discrete geometries were calculated here with $t = 6.67 \mu\text{m}$, $w_s = 7 \mu\text{m}$, $w = 42 \mu\text{m}$, $L = 132 \mu\text{m}$, $R = 116 \mu\text{m}$, and $L_{\text{und}} = 27 \mu\text{m}$ —the line is simply a guide for the eye. The FEM calculated mode shapes correspond to the three extreme examples of the resonator design. The theoretical clamping loss limit $1/Q_{\text{th}}$ for nodal positioning is always finite with the geometry closest to this position (indicated by the arrow) yielding $1/Q_{\text{th}} \approx 2 \times 10^{-7}$.

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It is important to note that these various dissipation processes add incoherently such that the reciprocals of the corresponding Q -values satisfy $1/Q_{\text{tot}} = \sum_i 1/Q_i$, where the index i labels each mechanism. Thus, in a realistic setting, care must be taken to isolate the contribution under scrutiny. In contrast to damping mechanisms (i)-(iii) that exhibit various dependencies with external physical variables such as pressure and temperature, support-induced dissipation is a temperature and scale-independent phenomenon with a strong geometric character. This scale-independence implies that the same analysis can be applied to both micro- and nanoscale devices. Note that even if all other damping mechanisms have been mediated, support-induced damping poses a fundamental limit in Q , as the coupling between a suspended mechanical resonator and its supports cannot be avoided. Thus, this process remains significant in devices fabricated from high-quality materials operated in vacuum and at cryogenic temperatures, and is in fact unavoidable in any non-levitating system.

In this presentation we outline a FEM-enabled numerical solver for calculating the support-induced losses of a broad range of low-loss mechanical resonators. The efficacy of our approach is demonstrated via comparison with experimental results from monocrystalline resonators, specifically engineered in order to isolate support-induced losses, exploiting the unique geometric dependence of this mechanism. The efficiency of our numerical solver results from the use of a perturbative scheme that exploits the smallness of the contact area, based on the recently introduced “phonon-tunneling” approach [26]. This results in a significant simplification over previous approaches and paves the way for CAD-based predictive design of low-loss mechanical resonators.

2. Numerical Solver

We first introduce our numerical solver, which provides a new technique to efficiently model support-induced losses for a broad class of mechanical structures. Previous approaches have relied on either the direct solution of an elastic wave radiation problem involving the substrate [22-24,27] or the simulation of a perfectly absorbing artificial boundary [21,25], with applications typically limited to a few

specific geometries [20,21,25,27]. In contrast, our technique represents a substantial simplification in that it reduces the problem to the calculation of a perfectly decoupled resonator mode together with *free* elastic wave propagation through the substrate in the absence of the suspended structure. A key feature of our method is to combine a standard finite-element method (FEM) calculation of the resonator mode, allowing us to treat complex geometries as well as taking proper account of interference effects between the radiated waves.

In the phonon-tunneling picture the mechanical resonance of interest, characterized by frequency ω_R , is regarded as a phonon cavity that is weakly coupled to the exterior by a hopping process, whereby the elastic energy leaks out of the resonator through the narrow contact areas from which it is suspended [26]. Within this framework, one can start from the harmonic Hamiltonian associated with the elastic scattering eigenmodes of the structure, including the substrate, and derive a quantum model for the Brownian motion experienced by each resonance. The corresponding weak tunnel couplings can be obtained to lowest order in the small parameter $k_R d$, where $1/k_R$ is the characteristic length scale over which the resonator mode varies appreciably and d is the characteristic dimension of the contact area S from which the resonator is suspended. For typical structures that exhibit high- Q mechanical resonances, $k_R d \ll 1$ is comfortably satisfied. This justifies the weak coupling approximation and leads to a general expression for the associated dissipation $1/Q$ in terms of the overlaps between the scattering modes and the resonator mode. In the limit $d \rightarrow 0$ the leading contribution is obtained by replacing the scattering modes by the free modes of the supports, which yields the damping expressions outlined in Ref. 26.

Though the aforementioned framework is completely general, in order to investigate the predictive power of our approach, we focus specifically on the flexural modes of a symmetric plate geometry of thickness t that is inscribed in a circle of radius R , with the contact area S corresponding to the outer rim of an idealized circular undercut (undercut distance of L_{und}). In order to calculate the theoretical Q -values of such devices based on the general expressions developed previously, we have developed a FEM-based solver that determines the resonator

eigenmodes via an eigenfrequency analysis in COMSOL multiphysics and uses a decomposition into cylindrical modes for the support, which is approximated by the substrate modelled as an isotropic elastic half-space.

The latter approximation is expected to be quantitatively precise for the low-lying flexural resonances when the underetched gap between the suspended structure and the substrate satisfies $h < R$ (where h is the gap height), and the largest resonant wavelength for elastic wave propagation in the substrate is smaller than the relevant length scales characterizing the mounting of the sample. The aforementioned weak coupling condition, $k_R d \ll 1$, follows in this case from $t \ll R$. Extending the expressions developed in Ref. 26 for integration in a general FEM environment we thus obtain:

$$\frac{1}{Q} = \frac{\pi}{2\rho_s \rho_R \omega_R} \sum_{n,\gamma} \left| \frac{f_{z,n}}{c_\gamma^3} \right|^2 \tilde{u}_{n,\gamma} \left(\omega_R R / c_{\gamma,v_s} \right), \quad (1)$$

where we use cylindrical coordinates and introduce the dimensionless displacements and the linear stress Fourier components

$$\tilde{u}_{n,\gamma}(\tilde{q}, v_s) = 2\pi \int_0^{\pi/2} d\theta \sin \theta \left| \tilde{u}_{q,\gamma;z}^{(0)}(0, v_s) \right|^2 J_n^2(\tilde{q} \sin \theta)$$

with $n = 0, \pm 1, \pm 2, \dots$. Here $\gamma = l, t, s$ labels the relevant plane-wave modes $\tilde{u}_{q,\gamma;z}^{(0)}(r, v_s)$ of the half-space [28] [i.e. longitudinal (l), transverse SV (t), and surface acoustic waves (s) given that transverse SH waves do not contribute] with c_γ the corresponding speed of sound as determined by the density ρ_s (ρ_R), Poisson ratio v_s , and

Young's modulus E_s of the substrate (resonator). We adopt spherical coordinates for the incident wave vector \vec{q} with polar angle θ .

3. Experimental Study

For experimental verification of our solver, we have developed free-free micromechanical resonators consisting of a central plate of length L and width w suspended by four auxiliary beams as depicted in Fig. 1(a). These structures are etched from a high-reflectivity crystalline distributed Bragg reflector [29,30], suited for Fabry-Perot-based optomechanical systems [31], and utilize a free-free flexural design in which auxiliary beams with widths w_s and lengths L_s are placed at the nodes of the fundamental mode of the central resonator [17].

The free-free structures employed in this experimental effort provide an ideal platform to isolate and measure phonon tunneling dissipation: by altering the attachment position of the auxiliary beams, this design allows for a significant variation in geometry, while approximately preserving the frequencies and effective surface-to-volume ratios of the resonators. As these characteristics are kept constant, one can rule out the influence of additional damping mechanisms on the variation in Q and hence isolate support-induced losses. As expected, the minimum-loss design corresponds to the geometry in which the auxiliary beams are attached at the nodes of the fundamental resonance of the central resonator.

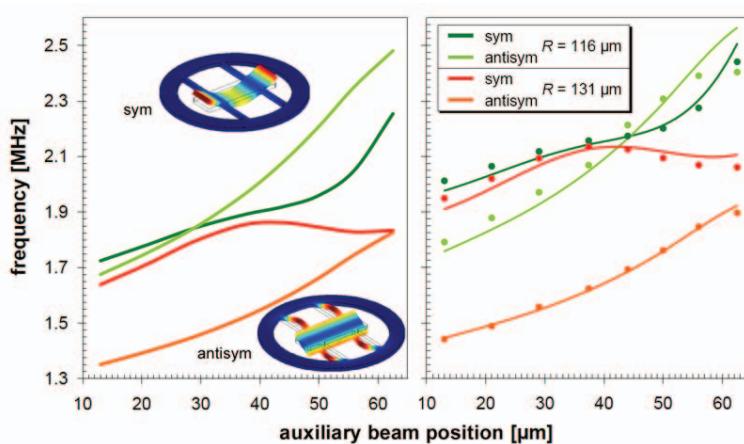


Figure 2. Simulated (left) and measured (right) eigenfrequencies as a function of the auxiliary beam y-coordinate. The measured values (discrete points) show excellent agreement with the simulated dataset, albeit with an offset dependent on the parity of the mode. The fitting lines in the right plot include a mean offset of 262 kHz for the symmetric free-free modes and 89 kHz for the antisymmetric modes (we attribute the shifts to a materials-related dissipation mechanism).

For mode identification we compare the optically measured resonator frequencies with the theoretical eigenfrequency response. The simulated values are generated using the geometric parameters determined via electron microscopy of the completed resonators. As can be seen in Fig. 2, in addition to the symmetric free-free resonance, there is also an antisymmetric eigenmode with comparable frequency. We observe no coupling between these resonances, which is consistent with the specific mirror symmetries of the structure.

All dissipation measurements have been performed in vacuum ($\sim 10^{-7}$ mbar) and at cryogenic temperatures (~ 20 K) in order to suppress fluidic and thermoelastic damping in the devices [32]. We record quality factors spanning 1.4×10^4 to 5.1×10^4 (cf. Fig. 3), with the minimum Q corresponding to the free-free mode of devices with an auxiliary position of $62.5\text{ }\mu\text{m}$ and $R = 116\text{ }\mu\text{m}$, and with the maximum Q to the geometry closest to nodal positioning ($37.4\text{ }\mu\text{m}$) for the same radius and type of mode. For the symmetric mode, we readily observe the expected characteristic modulation in Q as a function of the placement of the auxiliary beams with a relative variation of $\Delta Q_{\text{exp}}/Q_{\text{exp}} \approx 260\%$ ($\approx 80\%$) for $R = 116\text{ }\mu\text{m}$ ($R = 131\text{ }\mu\text{m}$). At the same time, the frequency variation is kept small *qua design*, with a range of $\Delta f/f \approx 20\%$ ($\approx 10\%$). In contrast, the Q -values for the antisymmetric mode are nearly constant with $Q \approx 2.1 \times 10^4$. This is expected as the theoretical support-induced loss for this mode is negligible. Additionally, as this resonance involves mainly deformations of the auxiliary beams, its dissipation is not expected to be correlated with the mode shapes of the central resonator. The damping of this mode is most likely dominated by the materials-related losses that are also responsible for the frequency shifts. We thus obtain an independent corroboration that the characteristic Q -variation observed for the free-free mode is induced by the modification of the geometry rather than by the small frequency variation present in the devices.

It is important to note that our model only captures support-induced losses, while other loss mechanisms may still contribute to the overall damping in the devices. However, given that we have designed sets of resonators for which the frequencies and effective surface-to-volume ratios are kept approximately constant, implies that any additional damping mechanism that is

relevant at low temperatures and high vacuum, but is insensitive to the variation in geometry, should contribute a constant offset $1/Q_*$ in the measured dissipation $1/Q_{\text{tot}}$.

Taking this offset into account, the theory shows remarkable agreement with the measured dissipation (Fig. 3). It is important to note that the only free parameter used here is a constant offset of $1/Q_* = 2.41 \times 10^{-5}$. Although the exact nature of the corresponding dissipation mechanism is currently unknown, we assume that it arises from materials losses in the resonator epi-structure. As our design isolates support induced-losses, these results establish the first systematic test of phonon tunneling dissipation in mechanical resonators.

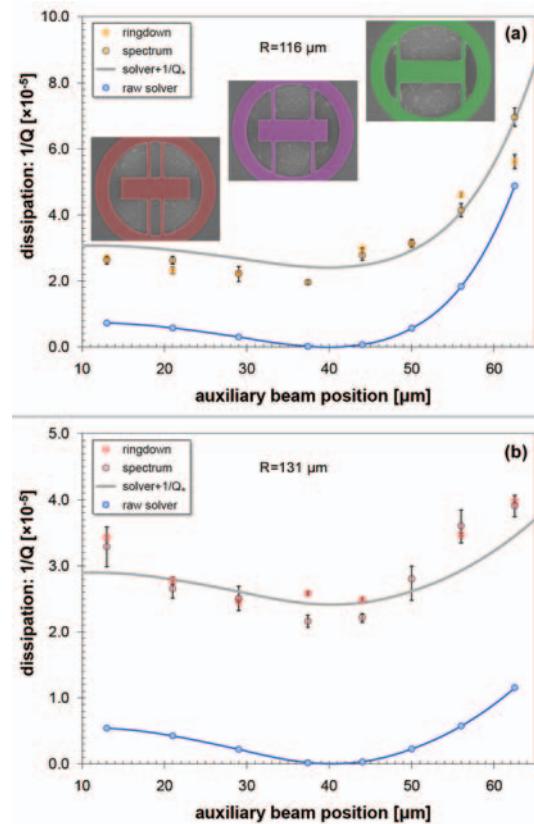


Figure 3. Compiled dissipation results displaying excellent agreement between theory and experiment. (a) and (b) Comparison of experimental measurements at $T = 20$ K with theoretical dissipation values for the free-free mode of resonators with measured central dimensions of $132\text{ }\mu\text{m} \times 42\text{ }\mu\text{m}$ and radius $R = 116\text{ }\mu\text{m}$ and $R = 131\text{ }\mu\text{m}$, respectively. Both ringdown and spectrally-derived data are included, with values averaged over two nominally-identical chips.

4. Conclusions

In conclusion, we have developed an efficient FEM-enabled solver for predicting the support-induced dissipation in micro- and nanoscale mechanical resonators. In combination with existing models for other relevant damping channels (e.g. fluidic and TED), our phonon-tunneling solver makes further strides towards accurate prediction of Q . Furthermore, we demonstrate a stringent experimental test of the corresponding theory using resonators engineered to isolate support-induced losses.

8. References

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